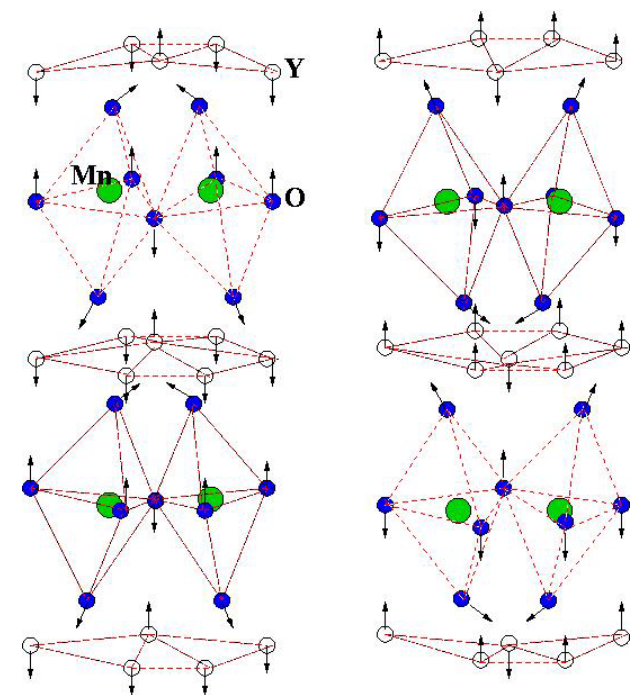




Computational design and optimization of novel multiferroics, Nicola Spaldin, UCSB, DMR-0312407

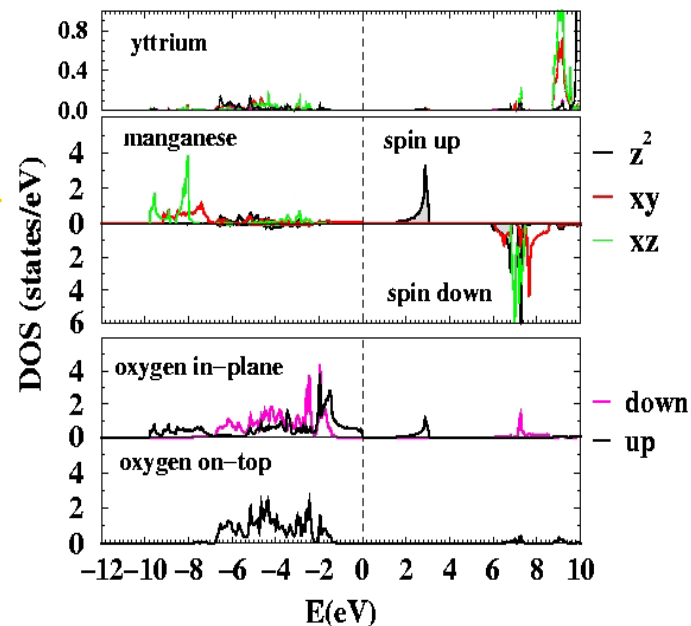


The Born Effective Charges, which are anomalously large in conventional ferroelectrics, are close to the formal ionic charges:

$$Y +3.6, Mn +3.3, O_T -2.3, O_P -2.2$$

- $YMnO_3$ is unusual and potentially technologically important because it combines ferroelectricity with magnetic ordering
- We determined that the ferroelectricity originates from geometric rotations, rather than the rehybridization that usually occurs at ferroelectric phase transitions
- Therefore usual indicators of ferroelectricity do not hold:

The density of states (DOS), calculated using our pseudopotential self-interaction corrected density functional formalism, indicates minimal Y-O and Mn-O hybridization



A. Filippetti and N.A. Spaldin, *Self-interaction-corrected pseudopotential scheme for magnetic and strongly-correlated systems*, Phys. Rev. B **67**, 125109 (2003)

B.B. van Aken, T.T.M. Palstra, A. Filippetti and N.A. Spaldin, *Origin of ferroelectricity in magnetoelectric $YMnO_3$* , Nature Materials **3**, 164 (2004)



Over 60 students from around the world worked with more than 15 teachers during the month-long school



A web-site:

<http://research.yale.edu/boulder/Boulder-2003>

was established with lecture notes, reading material, and other resources

Boulder School for Condensed Matter and Material Physics

PUBLIC LECTURE

A New Spin on Electronics

Stuart Parkin
Almaden Research Center, IBM Research

Conventional electronics depends only upon the charge of the electron. Electrons, however, also possess a property called "spin" -- it's where magnetism comes from. Until recently spin languished unused in the everyday world of electronics, but Spintronics puts electron spin back into the picture. Inventions based on this idea have already had dramatic effects on the home and office today.

Spinmeister Dr Stuart Parkin of the IBM Research Almaden Research Center will take you for a spin through this new field, discussing what spin is and why it matters, how it is being put to use today, and where you might find it tomorrow.

Thursday July 10, 7:30 pm
G1B20 Duane Physics Building, CU Campus

For information, call (303)-492-1515.
For Duane Building location, please consult the campus map.

Stuart Parkin is an IBM Fellow and manager of the Magnetolectronics Group at the IBM Almaden Research Center in San Jose, California. He is a leader in the rapidly growing field of spintronics, and his current work involves the study of magnetic tunnel junctions and the development of a new type of computer memory based upon them. More of his work is accessible on the web at www.research.ibm.com and www.almaden.ibm.com/st/



Public lectures were presented by Stuart Parkin (IBM) and Frances Hellmann (UCSD)

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